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Spin-boson systems : equivalence between the dilute-blip and the Born approximations

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Résumé. — Nous démontrons l'équivalence complète entre l'approximation des blips dilués introduite par Chakravarty et Leggett et l'approximation de Born du second ordre de la théorie générale de la relaxation. Outre sa simplicité, cette dernière approche permet de déduire directement la dynamique en utilisant l'analyse de Laplace standard. A titre d'exemple, le cas du double puits de potentiel symétrique est réexaminé. De plus, des expressions explicites de la coordonnée de la particule sont données pour certaines valeurs de la constante de couplage α , qui illustrent les trois cas : relaxation oscillante exponentiellement amortie ($\alpha < 1/2$), relaxation non exponentielle et non oscillante ($1/2 < \alpha < 1$) et finalement, dynamique au-dessus de la valeur critique ($\alpha > 1$).

Abstract. — We demonstrate the full equivalence between the dilute-blip approximation introduced by Chakravarty and Leggett, and the second-order Born approximation of the general relaxation theory. Besides its simplicity, the latter scheme allows us to derive the explicit dynamics in a direct way, invoking only standard analysis based on Laplace transformation. As an example, the case of the symmetric double-well potential is revisited. In addition, explicit expressions of the coordinate of the particle are derived for some values of the coupling constant α , which serve as illustrations of the three cases : exponentially damped oscillatory relaxation ($\alpha < 1/2$), non-exponential and non-oscillatory relaxation ($1/2 < \alpha < 1$) and finally, dynamics above the critical value ($\alpha > 1$).

In this paper we demonstrate the equivalence between the dilute blip approximation introduced by Chakravarty and Leggett [1], and subsequently used by many authors (see e.g. [2]), and the standard second-order Born approximation. We shall consider the case of a particle in a symmetric double-well potential, and linearly coupled to a bath of phonons.

Our aim is essentially to show that, at the level of approximation considered in almost all papers devoted to quantum ohmic dissipation, only plain relaxation theory and usual analysis are required.

The particle-plus-bath system is, as usual [1-3], represented by the coupled spin-boson Hamiltonian :

$$\hbar^{-1} H = - (\omega_0/2) \sigma_x + \sigma_z \sum_n G_n (b_n + b_n^\dagger) + \sum_n \omega_n b_n^\dagger b_n + \text{Cte} . \quad (1)$$

with an obvious notation. As quoted by Harris and Silbey [4] and Zwerger [5], the following unitary transformation S almost completely diagonalizes the Hamiltonian except for the tunnelling term proportional to ω_0 :

$$S = \exp \left[\sigma_z \sum_n \left(G_n / \omega_n \right) (b_n^\dagger - b_n) \right] . \quad (2)$$

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The transformed Hamiltonian $H' = S^+ H S$ now reads :

$$\begin{aligned} \hbar^{-1} H' &= - \left(\omega_0/2 \right) \left(B_+ \sigma_+ + B_- \sigma_- \right) + \sum_n \omega_n b_n^+ b_n \\ &\equiv H_{\text{int}} + H_0. \end{aligned} \quad (3)$$

The bath operators B_{\pm} are defined as $\exp \left[\pm 2 \sum_n \left(G_n / \omega_n \right) \left(b_n - b_n^+ \right) \right]$. The operator σ_z , which pictures the particle coordinate, is clearly invariant by the transformation S . We now follow the same lines as in general relaxation theory [6] ; first we define a set of four orthonormal operators, σ_{μ} , for the particle, made up with the 2×2 normalized unit operator 1_{particle} and three normalized Pauli matrices such that $\text{Tr} \left(\sigma_{\mu}^+ \sigma_{\mu'} \right) = \delta_{\mu\mu'}$. By a formal elimination of the bath operators in the coupled equations of motion, each of the σ_{μ} 's is seen to obey an equation of the type :

$$d\sigma_{\mu}/dt = e^{iQLt} P \sigma_{\mu}(t) - \sum_{\mu'} \int_0^t dt' \sigma_{\mu}(t-t') \text{Tr} \left[\rho_{\text{bath}}(0) \sigma_{\mu'}^+ L_{\text{int}} e^{iQLt'} L_{\text{int}} \sigma_{\mu'} \right]. \quad (4)$$

In this equation, the L 's are the Liouvillians associated to the H 's in equation (3). P is the projector $1_{\text{bath}} \rho_{\text{bath}}(0)$ and $Q = 1 - P$. The first term in the r.h.s. of equation (4) represents the fluctuating Langevin force, whereas the second one accounts for the dissipation. The mean value of σ_{μ} can now be obtained by averaging equation (4) over the total initial density operator, which we assume as usual to be factorized. Since the relaxation term in equation (4) already involves two interactions, we replace L by L_0 in the propagator : this is the second-order Born approximation. A simple calculation now yields :

$$(d/dt) \sigma(t) = - \omega_0^2 \int_0^t K(t-t') \sigma(t') dt' \quad (5)$$

where $\sigma(t)$ simply denotes the average value of σ_z . The retarded kernel $K(t)$ is the mean value of the anticommutator of the B 's :

$$K(t) = (1/2) \left\langle \left\{ B_+, B_-(t) \right\} \right\rangle. \quad (6)$$

In this equation, the average is taken on the canonical bath at temperature $T = 1/k_B \beta$. Equations (5) and (6) can be derived for any coupling of the form (3), provided that the mean values $\langle B_{\pm} \rangle$ vanish. This is indeed the case for the dissipation models defined by setting : $\rho(\omega) |G(\omega)|^2 = (\alpha/2) (\omega^{\delta}/\omega_c^{\delta-1}) f(\omega/\omega_c)$ for $\delta \leq 1$ where f is a cut-off function ($f(0) = 1$) having no bearing on the dynamics for times $\geq \omega_c^{-1}$. The value $\delta = 1$ corresponds to the so-called ohmic model which has been recently extensively studied.

Equation (5) can now be formally integrated to give the infinite series ($\Sigma(t) = \sigma(t)/\sigma(0)$) :

$$\Sigma(t) = \sum_{n=0}^{\infty} \left(-\omega_0^2 \right)^n \int_0^t \int_0^{t_1} \dots \int_0^{t_{2n-1}} K(t_1-t_2) K(t_3-t_4) \dots K(t_{2n-1}-t_{2n}) \prod_i dt_i. \quad (7)$$

Expression (7) is exactly the same as that given in references [1-3] with the same kernel K . Indeed, by taking an exponential cut-off function as in the latter articles, $K(t)$ for the ohmic case is equal to $\cos A_1(t) \exp[-A_2(t)]$ with :

$$A_1(t) = \cos \left[2 \alpha \tan^{-1} \left(\omega_c t \right) \right] \quad (8)$$

$$A_2(t) = \alpha \ln \left[1 + \left(\omega_c t \right)^2 \right] + 2 \alpha \sum_{n=1}^{\infty} \ln \left\{ 1 + \left[\omega_c t / \left(1 + n\beta \hbar \omega_c \right) \right]^2 \right\}.$$

This establishes the desired equivalence, as far as σ is concerned.

In the appendix, we explicitly derive the dynamics of $\sigma(t)$ at all relevant times by means of a standard Laplace analysis. Closed new expressions for $\sigma(t)$ are given in the three regimes : underdamped, overdamped (for α below its critical value $\alpha = 1$), and localized ($\alpha > 1$).

In order to be complete, one should discuss the conditions of validity of equation (6), which results from the truncation of the perturbation series. Roughly speaking, such an approximation is hoped to be valid when $\omega_0 \tau_c \ll 1$, where τ_c is some correlation-time of the reservoir ; this provides a reasonable validity criterion. A more precise delineation of the range of validity would imply a thorough study of the convergence of the perturbation series, a rather formidable task, in view only of the first (unwritten above) neglected term.

In this paper, our aim was essentially to show that the sophisticated and beautiful calculations using functional integration based on the so-called dilute blip approximation [1-3], can be reformulated in terms of plain relaxation theory, namely the « second-order » Born approximation. The preliminary unitary transformation S has a clear physical meaning : it merely expresses that every oscillator of the bath, due to its coupling with the particle, is shifted by a quantity depending on the particle coordinate. We believe that our method, besides its simplicity, is more transparent from a physical point of view ; anyway, it offers an alternate equivalent

scheme avoiding heavy calculations with a non-trivial physical meaning.

The equivalence has just been displayed in the case of a particle in a double-well coupled with phonons in an ohmic way ; we believe that it still stands for less specific models with other potentials. Indeed, one can convince oneself that this equivalence essentially relies on the underlying algebraic structures of both schemes, not on the peculiar details specific of a given physical system. In a forthcoming paper, we will give a detailed analysis for the non-ohmic case. We also intend to discuss the conditions of validity of the time-convolution equation of motion as compared to the time-convolution-less formalism [7] along the lines developed by Van Kampen [8].

Appendix.

The calculation of $\sigma(t)$ is obviously most easily achieved by taking the Laplace transform of equation (5) (not by considering its integrated form (7)) ; for simplicity, we shall only consider here the zero-temperature limit and the ohmic dissipation case ; setting $\Sigma_L(z)$:

$$\Sigma_L(z) = \int_0^{+\infty} e^{-z\omega t} \Sigma(t) d(\omega_c t) \quad (A.1)$$

one readily obtains ($g = \omega_0/\omega_c$) :

$$\Sigma_L(z)^{-1} = z + g^2 \times \left\{ z^{2\alpha-1} \cos(\alpha\pi + z) \Gamma(1-2\alpha) + \sum_{n=0}^{\infty} (1/n!) (-z)^n [\sin(z + n\pi/2)] / (n - 2\alpha + 1) \right\} \quad (A.2)$$

This expression is valid for all α ; (for $\alpha =$ integer or half-integer, the appropriate limits have to be carefully taken. Γ denotes the Euler function). The essential feature of Σ_L is the existence of the multi-valued function $z^{2\alpha-1}$ the cut of which is, for convenience, defined on the real negative axis ; on the other hand, the infinite series appearing in equation (A.2), denoted as $S(z)$ in the following, has no singularity for any finite z .

The Laplace transformation can now be inverted by using a contour made up with the two semi-infinite lines on both sides of the cut (from $-\infty - i0$ to $0_- - i0$ and from $0_+ + i0$ to $+\infty + i0$), joined together by a small anticlockwise circle γ around the origin, giving the J_γ term below. By doing so, one finds :

$$\Sigma(t) = [-g^2/\Gamma(2\alpha)] I(\alpha; t) + J_\gamma(\alpha) + \sum \text{Res} \quad (A.3)$$

$I(\alpha; t)$ is the integral :

$$I(\alpha; t) = \int_0^{+\infty} dx e^{-\omega dx} x^{2\alpha-1} \cos(\alpha\pi - x) / D(x) \quad (A.4)$$

with :

$$D(x) = [x - g^2 S(-x)]^2 + 2g^2 \cos(\alpha\pi - x) \Gamma(1-2\alpha) x^{2\alpha-1} [x - g^2 S(-x)] + g^4 [\cos(\alpha\pi - x) \Gamma(1-2\alpha)]^2 x^{2(2\alpha-1)}. \quad (A.5)$$

The $\sum \text{Res}$ includes all residues related to the poles located in the first Riemann sheet (defined such that $z^{2\alpha-1}$ takes on real positive values on the positive real axis) ; all of them have a negative real part (see below). The J_γ is clearly the only time-independent term (moreover all others vanish at infinite times) and therefore yields the value of $\Sigma(+\infty)$. A numerical calculation of $\Sigma(t)$ is very easy to achieve but all the essential results can be analytically obtained.

As for the final value of Σ , one readily finds :

$$\Sigma(+\infty) = \begin{cases} 0 & \text{for } \alpha \leq 1 \\ 1/\left\{1 + (\omega_0/\omega_c)^2 / [(2\alpha-1)(2\alpha-2)]\right\} & \text{for } \alpha > 1. \end{cases} \quad (\text{A.6})$$

This expresses the well-known symmetry-breaking for any $\alpha > 1$. Furthermore, for times $\gg \omega_r^{-1}$ defined as :

$$\omega_r = \omega_c [g^2 \Gamma(1-2\alpha) \cos \alpha \pi]^{1/(2-2\alpha)} \quad (\text{A.7})$$

an asymptotic analysis of $I(\alpha; t)$ reveals that one has :

$$\begin{aligned} \Sigma(t) &\sim \Sigma(+\infty) - g^2 \cos \alpha \pi (\omega_c t)^{-2(\alpha-1)} & \text{for } \alpha > 1 \\ \Sigma(t) &\sim - (2/\pi) g^{-2} (1-2\alpha) \sin \alpha \pi (\omega_c t)^{-2(1-\alpha)} & \text{for } \alpha < 1. \end{aligned} \quad (\text{A.8})$$

The dynamics of Σ for $\omega_c t \gg 1$ only involves z values such that $|z| \ll 1$; by expanding the regular terms appearing in the denominator of $\Sigma_L(z)$ around the origin, the poles are easily found as the roots of the following equation :

$$z \left\{ 1 + g^2 / [(1-2\alpha)(2-2\alpha)] \right\} + g^2 \Gamma(1-2\alpha) (\cos \alpha \pi - z \sin \alpha \pi) z^{2\alpha-1} = 0 \quad (\text{A.9})$$

and, provided that $|\alpha - 1/2|$ or $|\alpha - 1|$ is larger than g^2 , this can be further simplified to give :

$$z^{2(1-\alpha)} + g^2 \Gamma(1-2\alpha) \cos \alpha \pi = 0. \quad (\text{A.10})$$

By following the above-defined branch of z^a , this equation is shown to have two conjugate poles, z_0 and z_0^* , such that :

$$z_0 = \exp \left[i \left(\omega_r / \omega_c \right) e^{i\alpha\pi / (2-2\alpha)} \right]. \quad (\text{A.11})$$

Equation (A.11) shows that these poles leave out the first Riemann sheet when α increases beyond $1/2$. This means that for $\alpha < 1/2$, $\Sigma(t)$ undergoes an exponentially underdamped oscillatory motion with the frequency $\omega_r \cos [\alpha \pi / (2-2\alpha)]$ and with the decay rate $\omega_r \sin [\alpha \pi / (2-2\alpha)]$. Above this value, $\Sigma(t)$ is just given by expression (A.3) where the term $\sum \text{Res}$ vanishes. A numerical calculation with the more exact equation (A.9) shows in fact that the threshold value is slightly less than $1/2$ and that, except in the close vicinity of $\alpha = 1/2$, the poles are given by equation (A.11) with a very great accuracy. The different behaviours (oscillating or non-oscillating) of Σ on either side of this threshold can be quickly seen by looking at $\Sigma_L(z=0+)$ (see Eq. (A.2)) which is exactly zero for $\alpha < 1/2$ and is infinite otherwise.

All the above results agree with those given in [1, 3] ; the P_{inc} term defined in these papers is to be interpreted as a small correction due to our replacement of the entire function $S(z)$ by its first few terms ; this correction is irrelevant for times $\gg \omega_c^{-1}$. Also note that these results exactly reproduce, in the limit $\alpha \rightarrow 0$, those obtained within a single-boson approximation [7].

The transient behaviour of Σ , for a definite $\alpha > 1/2$, can easily be numerically computed in any case ; however, for times $\gg \omega_c^{-1}$, a complete analytical calculation can be achieved for a set of values of α (of the form (positive odd-integer/4)) by using the Efrös theorem [9] ; note that this also includes $\alpha = 1/4$ which serves as a check of the above general results. For these values, and for the relevant times

$t \gg \omega_c^{-1}$, $\Sigma(t)$ can always be expressed with the help of the erf function $\Phi(z)$ [10] ; indeed, one has (setting $T = \omega_r t$) :

i) $\alpha = 1/4$.

$$\Sigma(T) = (1/3) e^T [1 - \Phi(T^{1/2})] + (2/3) e^{-T/2} \operatorname{Re} \left\{ e^{i\sqrt{3}T/2} [1 + \Phi(e^{i\pi/3} T^{1/2})] \right\} . \quad (\text{A.12})$$

For $\omega_r t \leq 1$, one essentially recovers the underdamped oscillatory motion, in agreement with the general result expressed by equation (A.11). On the contrary, for large times, expansion of the erf functions exactly reproduces the long time-tail given in equation (A.8).

ii) $\alpha = 3/4$.

In this case, we find the very simple expression :

$$\Sigma(t) = e^T [1 - \Phi(T^{1/2})] \quad (\text{A.13})$$

which again develops a long time-tail at large times. At intermediate times, the relaxation is non-oscillatory and clearly non-exponential.

iii) $\alpha = 5/4$.

This case exemplifies the behaviour of $\Sigma(t)$ above the critical value ; we find :

$$\Sigma(t) = \Sigma(+\infty) \{1 - e^T [1 - \Phi(T^{1/2})]\} \quad (\text{A.14})$$

Note that in this case, $\Sigma(t)$ is nearly a constant in time since $\Sigma(+\infty)$ is very close to 1 and since the relevant time scale is now extremely short (see Eq. (A.7) for $\alpha > 1$). In this respect, considering the dynamics for higher values of α is devoid of interest.

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